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Stable second-order finite-difference methods for linear initial-boundary-value problems

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Abstract

Finite-difference methods of second order at the boundary points are presented for problems with one-dimensional second-order hyperbolic and parabolic equations with mixed boundary conditions. These methods do not require information at points outside the region of consideration. The linear stability of the algorithms developed is investigated. Numerical experiments are given for illustrating the accuracy and stability of the methods. Though the focus is on homogeneous boundary conditions, finite-difference methods with non-homogeneous mixed boundary conditions are also developed. To show the potential of the methods developed, in terms of CPU time, a comparison is made with the Crank–Nicolson method.

Keywords: Mixed boundary conditions; Finite-difference methods; Stability

1. Introduction

Consider the second-order one-dimensional hyperbolic equation

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} + f(x,t), \qquad 0 < x < 1, \qquad t \geq 0 \tag{1}$$

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subject to the homogeneous mixed boundary conditions

$$\frac{\partial u(0,t)}{\partial x} - w_1 u(0,t) = 0, \qquad w_1 > 0, \qquad t \geq 0 \tag{2}$$

$$\frac{\partial u(1,t)}{\partial x} + w_2 u(1,t) = 0, \qquad w_2 > 0, \qquad t \geq 0 \tag{3}$$

and the initial conditions

$$u(x,0) = g_1(x), \qquad 0 < x < 1 \tag{4}$$

$$\frac{\partial u(x,0)}{\partial t} = g_2(x), \qquad 0 < x < 1. \tag{5}$$

Similarly, consider the one-dimensional parabolic equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \qquad 0 < x < 1, \qquad t \geq 0 \tag{6}$$

subject to the mixed boundary conditions (2) and (3) and the initial condition (4). Consider also the isothermal flow reactor with second-order reaction governed by the following parabolic equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - s\frac{\partial u}{\partial x} - ru^2, \qquad 0 < x < 1, \qquad t \geq 0 \tag{7}$$

subject to the boundary conditions

$$\frac{\partial u(0,t)}{\partial x} - su(0,t) = -s, \qquad s > 0, \qquad t \geq 0 \tag{8}$$

$$\frac{\partial u(1,t)}{\partial x} = 0, \qquad t \geq 0 \tag{9}$$

and the initial conditions

$$u(x,0) = 0, \qquad 0 \leq x \leq 1. \tag{10}$$

Note that the mixed boundary conditions (2), (3) and (9) are homogeneous, whereas the mixed boundary condition (8) is non-homogeneous. These types of differential equations occur frequently in many fields of science and engineering; see, for example, [1,2]. Finite-difference schemes of $O(h^p + k^2)$, where $p = 1$ or 2, at the boundary points and at the interior points, are well known in the literature; see [3]. In the present paper, stable and convergent finite-difference schemes are presented which offer truncation error $O(h^2 + k^2)$, where $h > 0$ is a space step and $k > 0$ is the time step, even at the boundary points. The finite-difference scheme for hyperbolic equations is explicit, three-level, uses five mesh points and is conditionally stable. That for parabolic equations is fully implicit, two-level and is A_0-stable. In Section 2, finite-difference methods are developed when the boundary conditions are homogeneous, that is, for the initial-boundary-value problems consisting of (1)–(6); in Section 3, stability and convergence of the second-order methods are established; in Section 4, the technique used in Section 2 to approximate $\frac{\partial^2 u}{\partial x^2}$ along the boundaries is extended to non-homogeneous boundary conditions to obtain a finite-difference method for the initial-boundary-value problem consisting of (7)–(10).

2. Derivation of the finite-difference methods

Let N be a positive integer, $h = 1/(N+1)$, let $x_l = lh$, $l = 0, 1, 2, \ldots, N+1$ and let $t_j = jk$, $j = 0, 1, 2, \ldots$. At the grid points (x_l, t_j), for notational simplicity, denote

$$u_l^j = u(x_l, t_j), \quad u_{xl}^j = \frac{\partial u(x_l, t_j)}{\partial x}, \quad u_{xxl}^j = \frac{\partial^2 u(x_l, t_j)}{\partial x^2}, \quad u_{xxxl}^j = \frac{\partial^3 u(x_l, t_j)}{\partial x^3},$$
$$u_{tl}^j = \frac{\partial u(x_l, t_j)}{\partial t}, \quad u_{ttl}^j = \frac{\partial^2 u(x_l, t_j)}{\partial t^2}, \quad f_l^j = f(x_l, t_j), \quad f_{xl}^j = \frac{\partial f(x_l, t_j)}{\partial x}, \quad \text{etc.}$$

Hyperbolic equations

At the grid point (x_0, t_j), the finite-difference scheme of truncation error $O(h + k^2)$ described in [3] (see last paragraph of page 30) is obtained as follows.

- Discretize the boundary condition (2) at (x_0, t_j), using a central-difference approximation to u_x resulting in a fictitious point u_{-1}^j being introduced.
- Use the above value of the fictitious point, u_{-1}^j, in the finite-difference method written at (x_0, t_j).

Hence, in the above method it is assumed that (a) the differential equation (1) is valid along the boundaries, (b) the unknown function $u(x, t)$ is differentiable a sufficient number of times, (c) the Taylor series is valid about the points (x_0, t_j). Hence, without any loss of generality, at the grid point (x_0, t_j), the differential equation (1) can be written as

$$u_{tt0}^j = u_{xx0}^j + f_0^j. \tag{11}$$

Let

$$u_{xx0}^j = \alpha u_0^j + \beta u_1^j + \gamma u_{xxx0}^j. \tag{12}$$

Using the Taylor series for u_1^j about the point (x_0, t_j) in (12), and then equating the constant terms, and the coefficients of u_{xx0}^j and u_{xxx0}^j, gives

$$\alpha = -2(1 + hw_1)/h^2, \qquad \beta = 2/h^2, \qquad \gamma = -h/3. \tag{13}$$

Differentiating (1) and (2) at (x_0, t_j) with respect to x and t, respectively, and then using the assumption $u_{xtt0}^j = u_{ttx0}^j$, an expression for u_{xxx0}^j is obtained as

$$u_{xxx0}^j = w_1 u_{tt0}^j - f_{x0}^j. \tag{14}$$

Substituting (13) and (14) in (12) gives

$$u_{xx0}^j = \frac{\delta_x^2 u_0^j}{h^2} - \frac{h}{3} w_1 u_{tt0}^j + \frac{h}{3} f_{x0}^j, \tag{15}$$

where

$$\delta_x^2 u_0^j = -2(1 + hw_1) u_0^j + 2u_1^j.$$

Substituting (15) in (11) and then using the approximation $u_{tt0}^j = \frac{\delta_t^2 u_0^j}{k^2}$ gives

$$\left(\left(1 + \frac{hw_1}{3} \right) \delta_t^2 - r_h^2 \delta_x^2 \right) u_0^j = k^2 (F_0^j + f_0^j) + k^2 T_0^j \tag{16}$$

where

$$\delta_t^2 u_0^j = u_0^{j+1} - 2u_0^j + u_0^{j-1}, \qquad F_0^j = \frac{h}{3} f_{x0}^j, \qquad r_h = \frac{k}{h}$$

and

$$T_0^j = \left(1 + \frac{hw_1}{3}\right) \frac{k^2}{12} u_{tttt0}^j - \frac{h^2}{12} u_{xxxx0}^j.$$

The terms r_h and T_0^j are, respectively, the mesh ratio parameter for hyperbolic equations and the principal part of the local truncation error at (x_0, t_j).

Similarly, the scheme at (x_{N+1}, t_j) is derived as

$$\left(\left(1 + \frac{hw_2}{3}\right) \delta_t^2 - r_h^2 \delta_x^2\right) u_{N+1}^j = k^2 (F_{N+1}^j + f_{N+1}^j) + k^2 T_{N+1}^j, \tag{17}$$

where

$$F_{N+1}^j = \frac{-h}{3} f_{xN+1}^j, \qquad \delta_x^2 u_{N+1}^j = 2(u_N^j - (1 + hw_2) u_{N+1}^j),$$
$$T_{N+1}^j = \left(1 + \frac{hw_2}{3}\right) \frac{k^2}{12} u_{ttttN+1}^j - \frac{h^2}{12} u_{xxxxN+1}^j.$$

The derivation for $l = 1, 2, \ldots, N$ is seen in Smith [3] and is given by

$$(\delta_t^2 - r_h^2 \delta_x^2) u_l^j = k^2 (F_l^j + f_l^j) + k^2 T_l^j, \tag{18}$$

where

$$F_l^j = 0, \qquad \delta_x^2 u_l^j = u_{l-1}^j - 2u_l^j + u_{l+1}^j \qquad \text{and} \qquad T_l^j = \frac{k^2}{12} u_{ttttl}^j - \frac{h^2}{12} u_{xxxxl}^j.$$

It is easy to see that, for $l = 0(1)N + 1$, $T_l^j = O(k^2 + h^2)$ as $h, k \to 0$. Eqs. (16)–(18) give the required finite-difference scheme for solving the hyperbolic equation (1). In matrix notation it can be written as

$$\boldsymbol{U}^{j+1} = (2I + r_h^2 A) \boldsymbol{U}^j - I \boldsymbol{U}^{j-1} + k^2 (\boldsymbol{F}^j + \boldsymbol{f}^j), \tag{19}$$

where $\boldsymbol{W}^{j+p} = [W_0^{j+p}, W_1^{j+p}, \ldots, W_{N+1}^{j+p}]^T$, $j = 0, 1, 2, \ldots$, $p = 0$ or 1, and $\boldsymbol{W}$ may represent $\boldsymbol{U}$, $\boldsymbol{F}$ or $\boldsymbol{f}$ in (12). The matrix $A = [a_{i,j}]$ is a tridiagonal matrix of order $N + 2$ and is given by

$$A = \begin{pmatrix} \frac{-6(1+hw_1)}{3+hw_1} & \frac{6}{3+hw_1} & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & \frac{6}{3+hw_2} & \frac{-6(1+hw_2)}{3+hw_2} \end{pmatrix}. \tag{20}$$

2.1. Particular cases

(1) When $w_1 \to 0$, the values of the elements $a_{1,1}$ and $a_{1,2}$ in the matrix A are given by -2 and 2 respectively. From (19), the finite-difference scheme at (x_0, t_j) is

$$u_0^{j+1} = (2 - 2r_h^2)u_0^j + 2r_h^2 u_1^j - u_0^{j-1} + k^2\left(\frac{h}{3} f_{x0}^j + f_0^j\right). \tag{21}$$

To see that the finite-difference scheme given by (21) is consistent with the differential equation (1) at the grid point (x_0, t_j), rewrite (21) as follows:

$$\frac{u_0^{j+1} - 2u_0^j + u_0^{j-1}}{k^2} = \frac{-2u_0^j + 2u_1^j}{h^2} + \left(\frac{h}{3} f_{x0}^j + f_0^j\right). \tag{22}$$

When $w_1 \to 0$, the boundary condition (2) becomes $u_x(0, t) = 0$, which will give $u_{xtt}(0, t) = 0$ and $u_{xxx}(0, t) = -f_x(0, t)$. Hence, using $u_{x0}^j = 0$ and $u_{xxx0}^j = -f_{x0}^j$ in the Taylor series, about the point (x_0, t_j), of the functions in (22), the following equation is obtained.

$$u_{tt0}^j + O(k^2) = u_{xx0}^j + f_0^j + O(h^2). \tag{23}$$

As $h, k \to 0$, the above equation tends to the differential equation (1) at (x_0, t_j), which proves the consistency of the difference equation (19) at (x_0, t_j) as $w_1 \to 0$.

Similarly, when $w_2 \to 0$, the finite-difference scheme obtained from (19) at (x_{N+1}, t_j) is consistent with the differential equation (1) at (x_{N+1}, t_j).

(2) When $w_1 \to \infty$, the boundary condition (3) becomes $u(x, t) = 0$. Hence no discretization is needed at (x_0, t_j). Consequently, the first difference scheme in (19) disappears. The corresponding matrix A is of order $N + 1$ and is obtained by deleting the first row and the first column of the matrix given in (20). Similar results hold true as $w_2 \to \infty$ or both $w_1, w_2 \to \infty$.

Parabolic equations

Using the same approximations $\delta_x^2 u_l^j$ given in Eqs. (16)–(18), the Crank–Nicolson method for solving the parabolic equation (6) may be written in the form

$$\left(I - \frac{r_p}{2} A\right) \boldsymbol{U}^{j+1} = \left(I + \frac{r_p}{2} A\right) \boldsymbol{U}^j \tag{24}$$

where $r_p = \frac{k}{h^2}$, is the mesh ratio for parabolic equations and the matrix A is defined as in (20).

3. Stability and convergence

The aim of this section is to obtain a valid stability criterion for the difference scheme given by (19) and (24). The scheme (19) can be written in two-time-level form as

$$\begin{aligned} \boldsymbol{U}^{j+1} &= (2I + r_h^2 A)\boldsymbol{U}^j - \boldsymbol{V}^j + k^2(\boldsymbol{F}^j + \boldsymbol{f}^j), \\ \boldsymbol{V}^j &= \boldsymbol{U}^j, \end{aligned} \tag{25}$$

so that the error vector $\boldsymbol{E} = \boldsymbol{u} - \boldsymbol{U}$ satisfies

$$\boldsymbol{E}^{j+1} = \begin{pmatrix} 2I + r_h^2 A & -I \\ I & O \end{pmatrix} \boldsymbol{E}^j. \tag{26}$$

For $l = 0(1)N + 1$, μ_l, the $2(N + 2)$ eigenvalues of the amplification matrix in (26), are determined from the $N + 2$ quadratic equations

$$\mu_l^2 - (2 + r_h^2\lambda_l)\mu_l + 1 = 0, \tag{27}$$

where λ_l, $l = 0(1)N + 1$, are the eigenvalues of the matrix A. The difference scheme (19) will be stable if $|\mu_l| \le 1$; that is, if

$$-4 \le r_h^2\lambda_l \le 0. \tag{28}$$

Applying Brauer's theorem, Ref. [3], to the matrix A, it is an easy task to verify that (a) the second inequality in (28) is satisfied for all values of r, (b) the first inequality is satisfied only if

$$r_h^2 \le \min\left\{\frac{2(3 + hw_1)}{3(2 + hw_1)}, \frac{2(3 + hw_2)}{3(2 + hw_2)}\right\}. \tag{29}$$

The inequality (29) is the required stability criterion for the finite-difference scheme (19). The scheme will be convergent as long as this stability criterion is satisfied.

It is seen that the difference scheme (24) for a parabolic equation is A_0-stable and convergent.

4. Finite-difference methods for isothermal reactor flow with second-order reaction

At the grid point (x_0, t_j), the differential equation (7) can be written as

$$u_{t0}^j = u_{xx0}^j - su_{x0}^j - r(u_0^j)^2.$$

Using the boundary condition (8), the above equation can be written as

$$u_{t0}^j = u_{xx0}^j - s^2(u_0^j - 1) - r(u_0^j)^2. \tag{30}$$

Let

$$u_{xx0}^j = \alpha u_0^j + \beta u_1^j + \gamma u_{xxx0}^j + \eta. \tag{31}$$

Proceeding as in Section 2, the values of α, β, γ, η and the expressions for u_{xxx0}^j and u_{xx0}^j are obtained as $\alpha = \frac{-2(1+hs)}{h^2}$, $\beta = \frac{2}{h^2}$, $\gamma = \frac{-h}{3}$, $\eta = \frac{2s}{h}$, $u_{xxx0}^j = su_{t0}^j + su_{xx0}^j - 2rsu_0^j(1 - u_0^j)$, $u_{xx0}^j = \frac{3}{3+hs}(\frac{-2(1+hs)}{h^2}u_0^j + \frac{2}{h^2}u_1^j - \frac{hs}{3}u_{t0}^j + \frac{2hrs}{3}u_0^j(1 - u_0^j)) + \frac{6s}{h(3+hs)}$. Substituting this expression of u_{xx0}^j in (30) and following the techniques used in the Crank–Nicolson method (see [2]), a finite-difference scheme at $(x_0, t_{j+\frac{1}{2}})$ is obtained which is given by

$$\left(\frac{1}{k} + \frac{r}{2}u_0^{j+\frac{1}{2}} + a\right)u_0^{j+1} - bu_1^{j+1} = \left(\frac{1}{k} - \frac{r}{2}u_0^{j+\frac{1}{2}} - a\right)u_0^j + bu_1^j + c(u_0^j)^2 + d, \tag{32}$$

where $a = \frac{6+6sh+3s^2h^2+h^3(s^3-2rs)}{2h^2(3+2hs)}$, $b = \frac{3}{h^2(3+2hs)}$, $c = \frac{-rsh}{3+2hs}$, $d = \frac{6s+3s^2h+s^3h^2}{h(3+2hs)}$, and $u_0^{j+\frac{1}{2}} = u_0^j + \frac{k}{2h^2(3+2hs)}(a_1u_0^j + 6u_1^j + a_2(u_0^j)^2 + a_3)$ with $a_1 = -6(1 + hs) - s^2h^2(3 + hs) + 2h^3rs$, $a_2 = -3rh^2(1 + hs)$, $a_3 = 6sh + h^2s^2(3 + hs)$.

Similarly, the finite-difference scheme at (x_{N+1}, t_j) is obtained which is given by

$$pu_N^{j+1} + \left(\frac{1}{k} + \frac{r}{2}u_{N+1}^{j+\frac{1}{2}} - p\right)u_{N+1}^{j+1} = -pu_N^j + \left(\frac{1}{k} - \frac{r}{2}u_{N+1}^{j+\frac{1}{2}} + p\right)u_{N+1}^j, \tag{33}$$

where $p = \frac{-3}{h^2(3-hs)}$ and $u_{N+1}^{j+\frac{1}{2}} = u_N^j + \frac{3k}{h^2(3-hs)}(u_N^j - u_{N+1}^j - q(u_{N+1}^j)^2)$, with $q = \frac{rh^2(3-hs)}{6}$. At an interior point (x_l, t_j), the Crank–Nicolson method given in [2] is used.

5. Numerical illustrations

Example 1. To illustrate the second-order convergence of the scheme (19), the hyperbolic equation (1) is solved with $w_1 = 0.6, w_2 = 0.9079$ in (2) and (3), respectively. The average relative error percentage **(AREP)** and order are tabulated in Table 1 at $t = 2.0$ with $r_h = 0.4$. The table of values shows the second-order convergence. The exact solution $u(x,t)$ and the solution at the first-time level $u(x,k)$ are respectively given by $u(x,t) = [(x^2+1)(x+\frac{1}{4})\exp(-x) + \cos(x)]\exp(-t)$ and $u(x,k) = g_1(x) + kg_2(x) + \frac{k^2}{2}g_{1_{xx}}(x)$. The values of w_1 and w_2 are chosen in such a way that the boundary conditions (2) and (3) are satisfied with the exact solution, $u(x,t)$, given above.

Example 2. To illustrate the convergence of the scheme (24), consider the parabolic equation (6) with boundary conditions $u(0,t) = 1$ and $\frac{\partial u(1,t)}{\partial x} + w_2 u(1,t) = 0$, where $w_2 = (1-r)/r$, in which $r = 0.999$. The theoretical solution of the above problem is given by equations (30), (31) and (113) in the papers [1] and [4]. Comparing the computed solution obtained from the numerical scheme (24) at $t = 0.4$ with the theoretical solution, **AREP** and order are tabulated in Table 1 with $k = 0.001$. The results illustrate the convergence of the method. The order of the method is computed using Algorithm 1. When the order of a method increases as h decreases, it can be considered as a bonus to the convergence.

Algorithm 1.

Algorithm to evaluate the order

- Input: m, the number of values that h takes. (In the above table $m = 4$, as h takes four values.)
- Input: $AREP1$, the average relative error percent with current value of h. (In the first example, $AREP1 = 8.29e-01$.)
- DO $i \leftarrow 1$ to $m-1$
  - Input: $AREP2$, the average relative error percentage, with step size $\frac{h}{2}$
  - Order $\leftarrow \frac{\log(\frac{AREP1}{AREP2})}{\log(2)}$
  - Output: Order
  - $h \leftarrow \frac{h}{2}$
  - $AREP1 \leftarrow AREP2$
- END DO i

Example 3. Consider the isothermal flow reactor with second-order reaction governed by Eqs. (7)–(10). The values of the parameters given in [2] are $s = 10$ and $r = 5$. In [2], this engineering problem is solved using the Crank–Nicolson method at the mesh points (x_l, t_j), where $x_l = (l - \frac{1}{2}h)$, $h = 0.05$, $l = 1(1)20$ and $j = 1(1)40$. Varying time steps, k_j, are used and the values of t_j are given by $t_j = t_{j-1} + k_{j-1}$, with

Table 1
Numerical results for Example 2

Example 1			Example 2		
h	**AREP**	Order	h	**AREP**	Order
$\frac{1}{4}$	8.29e−01	–	$\frac{1}{5}$	1.07e−02	–
$\frac{1}{8}$	2.07e−01	2.00	$\frac{1}{10}$	1.82e−03	2.55
$\frac{1}{16}$	5.16e−02	2.00	$\frac{1}{20}$	3.29e−04	2.47
$\frac{1}{32}$	1.29e−02	2.00	$\frac{1}{40}$	3.59e−05	3.20

$t_0 = 0$, $k_0 = h^2$ and $k_j = 1.1k_{j-1}$, $j = 1(1)40$. The values of $u(x, t)$ along the boundaries are evaluated as the average of the exterior value and the first neighbouring interior value.

The above problem is solved using the schemes given in Section 4, with the same values of t_j and with $x_l = lh$, $l = 0(1)20$. In both cases, the steady-state temperature is reached after 39 iterations. The steady-state solutions in the intervals $0 \leq x \leq 1$ and $0 \leq x \leq 0.1$, respectively, are given in (a) and (b) of Fig. 1. From (b) of Fig. 1, note that the solution obtained by the proposed method is smooth near to the boundary $x = 0$, whereas that obtained by the Crank–Nicolson method is non-smooth. As the value of h decreases, the solution obtained by the Crank–Nicolson method approaches the solution obtained by the proposed method with $h = 0.05$. In this way, the maximum improvement in the solution is obtained with $h = 0.01$ and the solution thus obtained in the interval $0 \leq x \leq 0.1$ is given in (c) of Fig. 1 along with the solution obtained by the proposed method with $h = 0.05$. The Crank–Nicolson method is implemented using the computer code given on page 68 of [2], and the same code is used to implement the proposed method, extending it to include the code for discretization along the boundary. The CPU time needed for the Crank–Nicolson method to obtain the solution given in (c) of Fig. 1 is seven times the CPU time needed for the proposed method to obtain the solution given in (c) of Fig. 1. Note that, even then, the Crank–Nicolson method does not achieve the smoothness of the solution near the boundary $x = 0$.

6. Summary

Second-order finite-difference methods at the boundary points have been developed for the numerical solution of second-order hyperbolic and parabolic differential equations with mixed boundary conditions and appropriate initial conditions. Numerical experiments confirm the order of the convergence. Though the focus is on homogeneous mixed boundary conditions, the method is extended to problems with non-homogeneous mixed boundary conditions, and tested on a non-linear problem.

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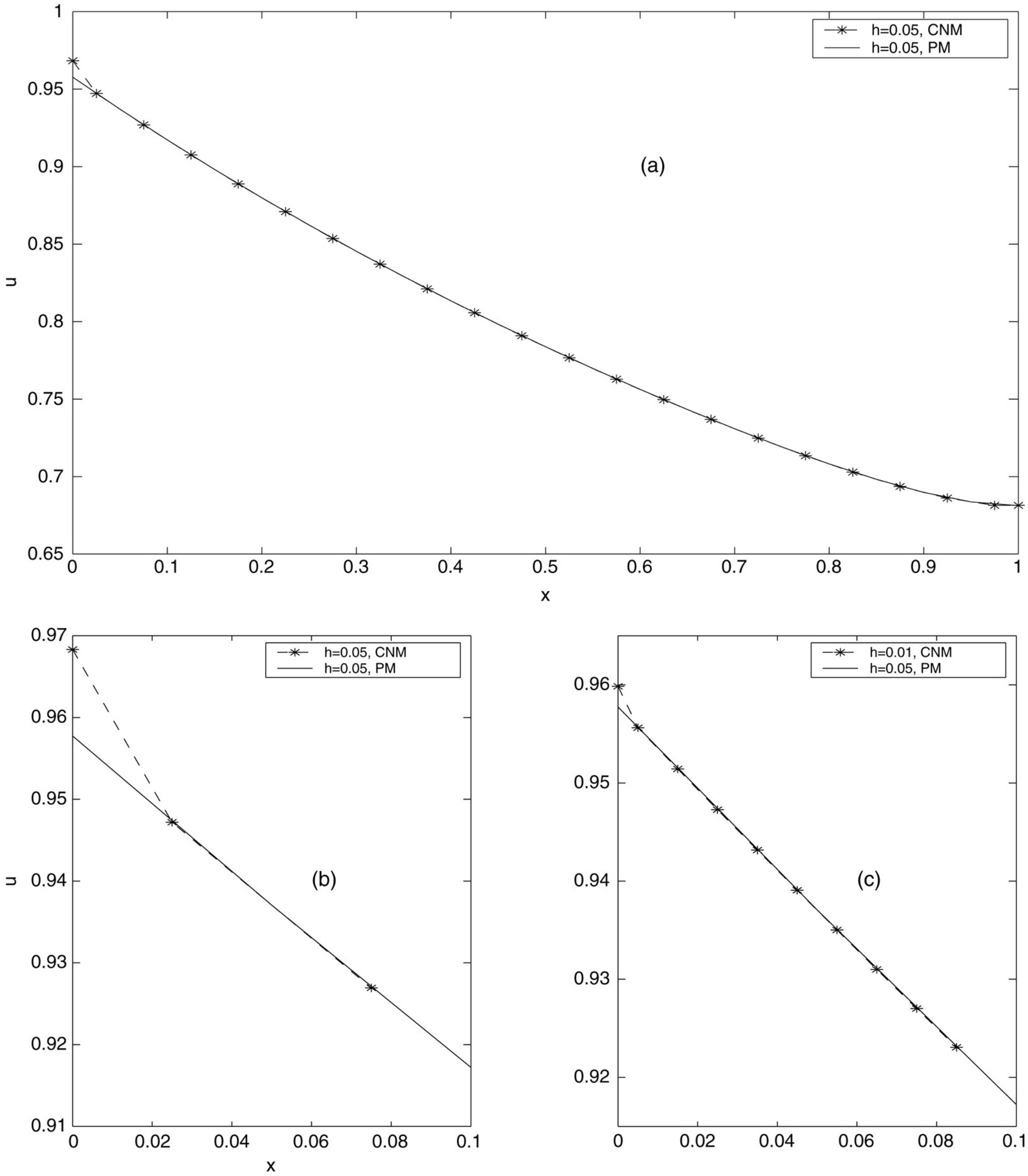

Fig. 1. Steady-state solution u versus x using the Crank–Nicolson Method (CNM) and the Proposed Method (PM).

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